Algorithmic and Theoretical Foundations of RL

Monte Carlo (MC) Learning

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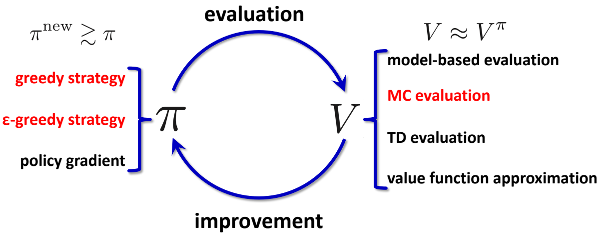
Policy Iteration Recap



Policy Iteration: greedy policy is improved via

$$\pi_{k+1}(s) = \arg\max_a \underbrace{\mathbb{E}_{s' \sim P(\cdot|s,a)}[r(s,a,s') + \gamma V^{\pi_k}(s')]}_{Q^{\pi_k}(s,a)},$$

where $V^{\pi_k}(s')$ is evaluated via Bellman equation based on the model.

— What if system information (P and r) is not available?

— Replace model by data (model free).

— How to collect data? How to use data?

— ......

MC Policy Evaluation (or Prediction)

Basic idea. Given π, estimate $V^\pi(s)$ and $Q^\pi(s,a)$ from sampled trajectories

$$\tau_i = \{(s_0^i, a_0^i, r_0^i, s_1^i, a_1^i, r_1^i, \cdots)\}_{i=1}^n \sim \pi.$$

- MC evaluation of $V^\pi(s)$: $s_0^i = s$,

$$V^\pi(s) \approx \frac{1}{n}\sum_{i=1}^n \left(\sum_{t=0}^\infty \gamma^t r_t^i\right).$$

- MC evaluation of $Q^\pi(s,a)$: $s_0^i = s$, $a_0^i = a$,

$$Q^\pi(s,a) \approx \frac{1}{n}\sum_{i=1}^n \left(\sum_{t=0}^\infty \gamma^t r_t^i\right).$$

Action Value Based Policy Iteration

- Policy improvement via state value:

$$\pi_{k+1}(s) = \operatorname*{argmax}_a \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[r(s,a,s') + \gamma V^{\pi_k}(s') \right].$$

  Given $V^{\pi_k}(s')$, still need to compute the expectation which requires model.

- Policy improvement via action value:

$$\pi_{k+1}(s) = \operatorname*{argmax}_a Q^{\pi_k}(s,a).$$

  Ideal for model free RL since we can estimate $Q^{\pi_k}(s,a)$ directly from data.

Primitive MC Learning Algorithm

Algorithm 1: Primitive MC Learning

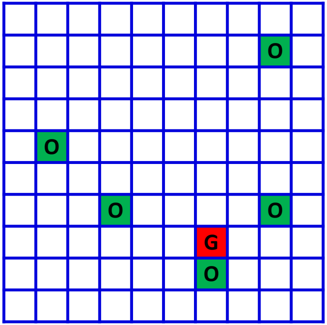
Initialization: π_0, n
for $k = 0, 1, 2, \ldots$ **do**
  for *every* s **do**
    for *every* a **do**
      Sample n episodes starting from (s, a), following π_k:

$$\tau_i = (s_0^i, a_0^i, r_0^i, s_1^i, a_1^i, r_1^i, \cdots, s_{T-1}^i, a_{T-1}^i, r_{T-1}^i, s_T^i) \sim \pi_k, \ \ i = 1, \cdots, n$$

      Compute $Q^k(s, a) = \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{t=0}^{T-1} \gamma^t r_t^i \right)$
    end
    $\pi_{k+1}(s) = \operatorname*{argmax}_a Q^k(s, a)$
  end
end

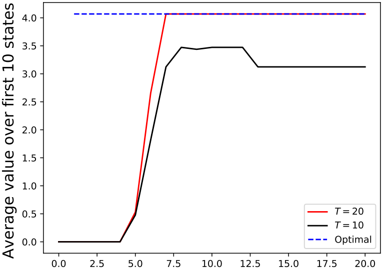
Ideally, T should be ∞ or s_T be a terminal state. In practice, T should be sufficiently large, especially for the sparse reward case.

Illustrative Example



Goal: +10, obstacle: -10; goal is terminal state.

Illustrative Example



The learned policy is evaluated exactly using model.

Inefficiency of Primitive MC Learning

- A trajectory is only used for estimating one state-action value;
- Wait until all trajectories have been collected before policy update;
- Old state-action values are not reused and thus wasted (next lecture).

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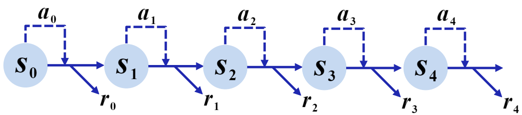
Use Trajectory More Efficiently



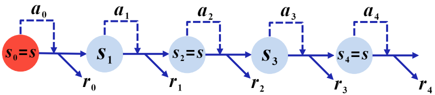
Trajectory $(s_0, a_0, r_0, s_1, a_1, r_1, \cdots) \sim \pi$ starting from s contains sub-trajectories $(s_t, a_t, r_t, s_{t+1}, a_{t+1}, r_{t+1}, \cdots)$ that starts from other states (e.g. $s_t = s'$). Thus, return from the sub-trajectory

$$G_t = \sum_{t'=t}^{\infty} \gamma^{t'-t} r_{t'}$$

can be used to build an estimator of $V^\pi(s')$. Namely, one trajectory can be used to estimate different $V^\pi(s)$.

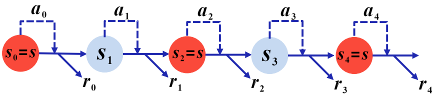
There is no essential difference in the MC evaluations of state value and action value in methodology. Thus discussion in this section will be mainly based on state value.

First-Visit and Every Visit



First Visit

- Only sub-trajectory that starts from the first visit of s is used in the estimation of $V^{\pi}(s)$; One trajectory is only used once in the evaluation of $V^{\pi}(s)$.



Every Visit

- All sub-trajectories that start from of s is used in the estimation of $V^{\pi}(s)$; One trajectory might be used many times in the evaluation of $V^{\pi}(s)$.

First-Visit MC Policy Evaluation

Algorithm 2: First-Visit Monte Carlo Policy Evaluation

Initialization: Counter of visited numbers $N(s) = 0$, the total return $G(s) = 0$, $\forall s \in \mathcal{S}$

for $k = 0, 1, 2, \ldots$ **do**

  Initialize s_0 and sample an episode following π:

$$(s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T) \sim \pi$$

  $G \leftarrow 0$

  for $t = T-1, T-2, \ldots, 0$ **do**

    $G \leftarrow \gamma G + r_t$

    if s_t *does not appear in* $(s_0, s_1, \cdots, s_{t-1})$ **then**

      $N(s_t) \leftarrow N(s_t) + 1$

      $G(s_t) \leftarrow G(s_t) + G$

      $V^{first}(s_t) \leftarrow G(s_t)/N(s_t)$

    end

  end

end

Every-Visit MC Policy Evaluation

Algorithm 3: Every-Visit Monte Carlo Policy Evaluation

Initialization: Counter of visited numbers $N(s) = 0$, the total return $G(s) = 0$, $\forall s \in \mathcal{S}$

for $k = 0, 1, 2, \ldots$ **do**

Initialize s_0 and sample an episode following π:

$$(s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T) \sim \pi$$

$G \leftarrow 0$

for $t = T-1, T-2, \ldots, 0$ **do**

$G \leftarrow \gamma G + r_t$

$N(s_t) \leftarrow N(s_t) + 1$

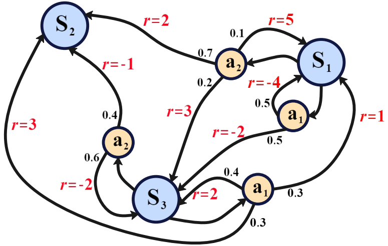
$G(s_t) \leftarrow G(s_t) + G$

$V^{every}(s_t) \leftarrow G(s_t)/N(s_t)$

end

end

Illustrative Example

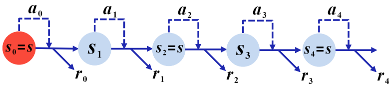


Consider policy $\pi(a|s) = 0.5$ for each state s and each action a and $\gamma = 0.9$. Recall that $V^{\pi} = [-0.21, 0, 0.31]^T$.

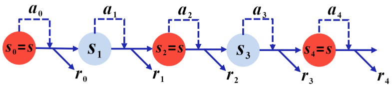
Consider a sampled trajectory: $(s_1, a_1, -2, s_3, a_1, 1, s_1, a_2, 3, s_3, a_2, -1, s_2)$.

- First-visit policy evaluation for state s_3:
  $N(s_3) = 1, V^{first}(s_3) = (1 + 0.9 \times 3 + 0.9^2 \times (-1)) = 2.89$.
- Every-visit policy evaluation for state s_3:
  $N(s_3) = 2, V^{every}(s_3) = (1 + 0.9 \times 3 + 0.9^2 \times (-1) - 1)/2 = 0.945$.

First-Visit vs Every-Visit



First Visit



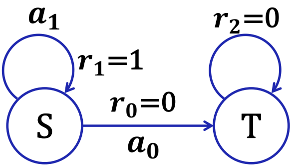
Every Visit

MSE = bias^2+variance

	Un-biased	Short MSE	Long MSE
First visit	Yes	Higher	Lower
Every visit	No	Lower	Higher

"Reinforcement learning with replacing eligibility traces" by Singh and Sutton, 1996.

Illustrative Example



$\pi(a_1|s) = p, \quad \pi(a_0|s) = 1-p$. Set $\gamma = 1$.

State value of π at s is $V^{\pi}(s) = \frac{p}{1-p}$.

- Single trajectory

$$\mathbb{E}\left[V^{first}(s)\right] = \frac{p}{1-p}, \quad \text{MSE}\left[V^{first}\right] = \text{Var}\left[V^{first}\right] = \frac{p}{(1-p)^2};$$
$$\mathbb{E}\left[V^{every}\right](s) = \frac{p}{2(1-p)}, \quad \text{MSE}\left[V^{every}\right] \leq \frac{p}{2(1-p)^2}.$$

- As the number of trajectories increases, it can be shown that

$$V^{every}(s) \to \frac{p}{1-p}.$$

Incremental Monte Carlo Policy Evaluation

As already seen, mean evaluation can be conducted in an incremental way:

$$N(s_t) \leftarrow N(s_t) + 1, \quad V(s_t) \leftarrow V(s_t) + \frac{1}{N(s_t)}(G - V(s_t)).$$

Algorithm 4: First-Visit Monte Carlo Policy Evaluation (Incremental Version)

Initialization: Visited numbers $N(s) = 0$ and initialize $V(s)\ \forall s \in \mathcal{S}$.

for $k = 0, 1, 2, \ldots$ **do**

  Initialize s_0 and sample an episode following π:

$$(s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T) \sim \pi$$

  $G \leftarrow 0$

  for $t = T-1, T-2, \ldots, 0$ **do**

    $G \leftarrow \gamma G + r_t$

    if s_t *does not appear in* $(s_0, s_1, \cdots, s_{t-1})$ **then**

      $N(s_t) \leftarrow N(s_t) + 1$

      $V(s_t) \leftarrow V(s_t) + \frac{1}{N(s_t)}(G - V(s_t))$

    end

  end

end

Without further specification, discussion in the rest of this lecture will focus on first visit, and the superscript "first" will be omitted.

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Simply Combine MC Policy Evaluation with Greedy Policy

Algorithm 5: MC Learning with Greedy Policy

Initialization: $Q(s, a) = 0, N(s, a) = 0, \forall s, a$; Initialize π_0.
for $k = 0, 1, 2, \ldots$ **do**
  Initialize s_0 and sample an episode following π_k:

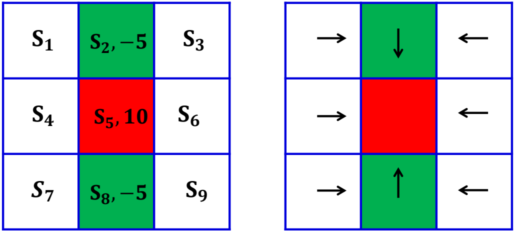
$$(s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T) \sim \pi_k$$

  $G \leftarrow 0$
  for $t = T-1, T-2, \ldots, 0$ **do**
    $G \leftarrow \gamma G + r_t$
    if (s_t, a_t) *does not appear in* $(s_0, a_0, s_1, a_1, \ldots, s_{t-1}, a_{t-1})$ **then**
      $N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$
      $Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \frac{1}{N(s_t, a_t)}(G - Q(s_t, a_t))$

$$\pi_{k+1}(a|s_t) = \begin{cases} 1 & \text{if } a = \operatorname*{argmax}_a Q(s_t, a) \\ 0 & \text{otherwise} \end{cases}$$

    end
  end
end

An Example Algorithm 5 Fails to Work



Consider the gridworld problem (left) where $\gamma = 0.9$. Assume $Q(s, a) = 0$ for all s, a and π_0 is given in the right plot. It can be verified that π_0 does not change for Algorithm 5.

Remark

How to collect data (or interaction with environment) is very important for success of RL algorithms. We mainly consider the following intersection protocol: Start from a state and then sample an episode following a policy (behavior policy). Eventually, we hope the data enables us to evaluate the action values of the target policy for all action pairs (recall that in model based policy iteration, action values are all equally evaluated for every action (full exploration) or the first action is independent of policy). However, the behavior policy may bias towards some actions , for example the greedy policy. On the one hand, collect data from a biased behavior policy may reduce the ability of exploration. One the other hand, if the behavior policy can provide good experiences, it should be able to provide good instruction to improve the target policy. Thus, there is a tradeoff between exploration and exploitation.

- How to encourage exploration?
  - Explore state-action pairs when sampling episodes.
  - ϵ-greedy policy
  - Off-policy learning

ϵ-Greedy Policy

With small probability ϵ randomly choose an action to ensure exploration:

$$\pi'(a|s) = \begin{cases} 1 - \epsilon + \frac{\epsilon}{|\mathcal{A}|} & \text{if } a = \operatorname*{argmax}_a Q^\pi(s, a'), \\ \frac{\epsilon}{|\mathcal{A}|} & \text{otherwise.} \end{cases}$$

Theorem 1

For any policy π, the ϵ-greedy policy π' with respect to Q^π is an improvement, i.e., $V^{\pi'}(s) \geq V^\pi(s)$, when ϵ is sufficiently small.

Proof of Theorem 1

It suffices to show the one-step improvement of π' over π: $\mathcal{T}^{\pi'} V^{\pi} \geq V^{\pi}$, which is equivalent to

$$\sum_a \pi'(a|s) Q^{\pi}(s,a) \geq \sum_a \pi(a|s) Q^{\pi}(s,a) = V^{\pi}(s).$$

This follows directly from

$$\begin{aligned}
\sum_a \pi'(a|s) Q^{\pi}(s,a) &= \frac{\epsilon}{|\mathcal{A}|} \sum_a Q^{\pi}(s,a) + (1-\epsilon) \max_a Q^{\pi}(s,a) \\
&= \frac{\epsilon}{|\mathcal{A}|} \sum_a Q^{\pi}(s,a) + \left(\sum_a \left(\pi(a|s) - \frac{\epsilon}{|\mathcal{A}|} \right) \right) \max_a Q^{\pi}(s,a) \\
&\geq \frac{\epsilon}{|\mathcal{A}|} \sum_a Q^{\pi}(s,a) + \sum_a \left(\pi(a|s) - \frac{\epsilon}{|\mathcal{A}|} \right) Q^{\pi}(s,a) \\
&= \sum_a \pi(a|s) Q^{\pi}(s,a).
\end{aligned}$$

MC Learning with ϵ-Greedy Policy

Algorithm 6: MC Learning with ϵ-Greedy Exploration

Initialization: $N(s,a) = 0, Q(s,a) = 0, \forall s, a$, π_0

for $k = 0, 1, 2, \dots$ **do**

  Initialize s_0 and sample an episode following π_k:

$$(s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T) \sim \pi_k$$

  $G \leftarrow 0$

  for $t = T-1, T-2, \dots, 0$ **do**

    $G \leftarrow \gamma G + r_t$

    if (s_t, a_t) *does not appear in* $(s_0, a_0, s_1, a_1, \dots, s_{t-1}, a_{t-1})$ **then**

      $N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$

      $Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \frac{1}{N(s_t, a_t)}(G - Q(s_t, a_t))$

      Update policy of visited state via ϵ_k-greedy:

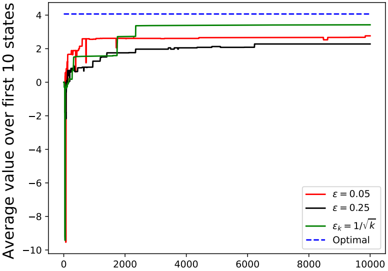
$$\pi_{k+1}(a|s_t) = \begin{cases} 1 - \epsilon_k + \frac{\epsilon_k}{|\mathcal{A}|} & \text{if } a = \operatorname*{argmax}_{a'} Q(s_t, a') \\ \frac{\epsilon_k}{|\mathcal{A}|} & \text{otherwise} \end{cases}$$

    end

  end

end

Illustrative Example



For the previously mentioned 10×10 gridworld problem.

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Off-Policy Monte Carlo Evaluation

- On-policy learning vs off-policy learning
  - On-policy: Learn target policy π from experience sampled from π;
  - Off-policy: Learn target policy π from experience sampled from *b*.
- On-policy ϵ-greedy method which is not deterministic needs to behave non-optimally in order to explore all actions.
- Off-policy method attempts to learn a deterministic optimal policy from data generated by another exploratory policy.

Importance Sampling for Off-Policy MC Evaluation

In order to evaluate action value $Q^\pi(s,a)$ from data sampled from a behavior policy b, we need to express $Q^\pi(s,a)$ in terms of the expectation with respect to b. Given a subtrajectory $\tau_t = \{s_t, a_t, r_t, s_{t+1}, a_{t+1}, r_{t+1}, \cdots\}$, let $(s_t, a_t) = (s, a)$ and P_t^π be the distribution of τ_t under policy π (similarly for P_t^b). We have,

$$
\begin{aligned}
Q^\pi(s,a) &= \mathbb{E}_{\tau_t \sim P_t^\pi}\left[G_t\right] \\
&= \mathbb{E}_{\tau_t \sim P_t^b}\left[\frac{P_t^\pi(\tau_t)}{P_t^b(\tau_t)} G_t\right],
\end{aligned}
$$

where $G_t = \sum_{t'=t}^{\infty} \gamma^{t'-t} r_{t'}$ and

$$
\frac{P_t^\pi(\tau_t)}{P_t^b(\tau_t)} = \frac{P(s_{t+1}|s_t,a_t)\prod_{k=t+1}^{\infty} P(s_{k+1}|s_k,a_k)\,\pi(a_k|s_k)}{P(s_{t+1}|s_t,a_t)\prod_{k=t+1}^{\infty} P(s_{k+1}|s_k,a_k)\,b(a_k|s_k)} = \prod_{k=t+1}^{\infty} \frac{\pi(a_k|s_k)}{b(a_k|s_k)}
$$

is known as importance-sampling ratio.

Importance Sampling for Off-Policy MC Evaluation

Given an

$$\{s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T\} \sim b,$$

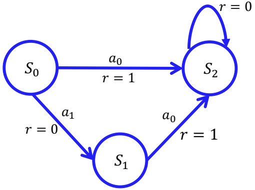
off-policy MC evaluation has the following form:

$$N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$$

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \frac{1}{N(s_t, a_t)} \left(G_t \frac{P_t^\pi}{P_t^b} - Q(s_t, a_t) \right)$$

Weight for Initial Pair Should Not Be Included

Note when defining $Q^{\pi}(s,a)$, action a is independent of policy π. Thus, when computing importance sampling weight for (s_t, a_t), $\frac{\pi(a_t|s_t)}{b(a_t|s_t)}$ is excluded.



Suppose $\gamma < 1$. Optimal policy for s_0 is $\pi^*(s_0) = a_0$. Set $Q(s,a) = 0$ for all (s,a), $\pi_0(s_0) = a_1$ and $\pi_0(s_1) = a_0$. Two possible episodes for an exploratory behavior policy b:

$$(s_0, a_0, 1, s_2) \quad \text{and} \quad (s_0, a_1, 0, s_1, a_0, 1, s_2).$$

It is easy to verify that π_0 will not be updated if $\frac{\pi_0(a_0|s_0)}{b(a_0|s_0)} = 0$ is included in the computation of importance sampling weight. In contrast, π_0 will be updated if $\frac{\pi_0(a_0|s_0)}{b(a_0|s_0)} = 0$ is not included.

Example is from Wenye Li.

Off-Policy MC Learning

Algorithm 7: Off-policy MC Learning

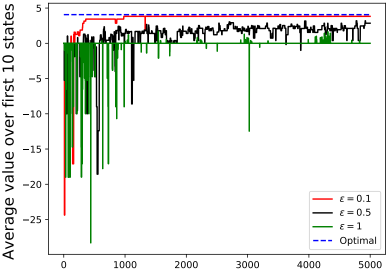
Initialization: $\forall s, a$, initialize $Q(s, a)$, $\pi_0(s) = \mathrm{argmax}_a\, Q(s, a)$, $N(s, a) = 0$.
for $k = 0, 1, 2, \dots$ **do**
  $b_k \leftarrow$ any soft policy, i.e., $b_k(a|s) > 0, \forall s, a$
  Initialize s_0 and sample an episode following b_k:

$$(s_0, a_0, r_0, s_1, a_1, r_1, \cdots, s_{T-1}, a_{T-1}, r_{T-1}, s_T) \sim b_k$$

  $G \leftarrow 0, W \leftarrow 1$
  for $t = T-1, T-2, \dots, 0$ **do**
    $G \leftarrow r_t + \gamma G$
    if (s_t, a_t) *does not appear in* $(s_0, a_0, s_1, a_1, \dots, s_{t-1}, a_{t-1})$ **then**
      $N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$
      $Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \frac{1}{N(s_t, a_t)}(W \cdot G - Q(s_t, a_t))$
      $\pi_{k+1}(s_t) \leftarrow \mathrm{argmax}_a\, Q(s_t, a)$
    end
    $W \leftarrow W \frac{\pi_k(a_t|s_t)}{b_k(a_t|s_t)}$
  end
end

To handle the potential high variance incurred by importance sampling, one may consider weighted importance sampling. See "Reinforcement learning: An introduction" by Sutton and Barto, 2018.

Illustrative Example



ϵ-greedy policy is used as behavior policy.

For the previously mentioned 10×10 gridworld problem.

Remark

- Policy evaluation and policy improvement is a general and fundamental framework for RL algorithms. Different evaluation methods may require different improvement methods, and vice versa. As already presented, if we use data sampled from target policy for evaluation, we should use ϵ-greedy policy for improvement to encourage exploration. In contrast, if using greedy policy for improvement, we may need to use data sampled from a more exploratory behavior policy for evaluation based on importance sampling.
- Most algorithms presented in this lecture and the next one admit certain convergence guarantees under mild conditions, details of which are omitted.

Questions?